The conserved operators generated by a solution of the Schrödinger equation

G.F. Torres del Castillo
Departamento de Física Matemática, Instituto de Ciencias,
Universidad Autónoma de Puebla, 72570 Puebla, Pue., México.

E. Navarro Morales
Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Puebla,
Apartado postal 1152 Puebla, Pue., 72001, México.

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It is shown that, in a similar manner as a complete solution of the Hamilton–Jacobi equation for a system with n degrees of freedom yields $2n$ constants of motion, each solution of the Schrödinger equation containing n parameters leads to $2n$ operators that are constants of motion; these $2n$ operators form two sets of n mutually commuting operators.

Keywords: Wavefunctions; Hamilton–Jacobi equation; Schrödinger's equation; constants of motion.

Se muestra que, en forma similar a como una solución completa de la ecuación de Hamilton–Jacobi para un sistema con n grados de libertad produce $2n$ constantes de movimiento, cada solución de la ecuación de Schrödinger que contenga n parámetros lleva a $2n$ operadores que son constantes de movimiento; estos $2n$ operadores forman dos conjuntos de n operadores que conmutan entre sí.

Descriptores: Funciones de onda; ecuación de Hamilton–Jacobi; ecuación de Schrödinger; constantes de movimiento.

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1. Introduction

One of the methods to find the solution of the equations of motion in classical mechanics is based on the Hamilton–Jacobi (HJ) equation (see, *e.g.*, Ref. 1). For a mechanical system with n degrees of freedom and Hamiltonian $H(q_i, p_i, t)$, the HJ equation is usually expressed as the partial differential equation

$$H\left(q_i, \frac{\partial S}{\partial q_i}, t\right) + \frac{\partial S}{\partial t} = 0. \tag{1}$$

Instead of looking for the general solution of this equation, one is interested in a *complete solution*, which is a function $S(q_1, \ldots, q_n, t, \alpha_1, \ldots, \alpha_n)$ satisfying the HJ equation, where the α_i are n arbitrary parameters. The function $S(q_1, \ldots, q_n, t, \alpha_1, \ldots, \alpha_n)$ is the generating function of a canonical transformation relating the original canonical coordinates p_i, q_i with a new system of canonical coordinates α_i, β_i which are all *constants of motion*. The transformation is given by

$$p_i = \frac{\partial S}{\partial q_i} \tag{2}$$

and

$$\beta_i = \frac{\partial S}{\partial \alpha_i}, \tag{3}$$

$i = 1, 2, \ldots, n$, provided that $\det(\partial^2 S/\partial q_i \partial \alpha_j) \neq 0$, so that Eqs. (3) can be (locally) inverted to give each q_i as some function of t and the $2n$ constants α_j, β_j; then, by substituting these expressions into Eqs. (2), the p_i are also given as functions of α_j, β_j, and t (see, *e.g.*, Ref. 1).

Since the β_i and α_i are canonical coordinates, their Poisson brackets are the same as those for the variables q_i, p_i (with α_i as the momentum conjugate to β_i)

$$\{\alpha_i, \alpha_j\} = 0, \quad \{\beta_i, \beta_j\} = 0, \quad \{\beta_i, \alpha_j\} = \delta_{ij}. \tag{4}$$

As is well known, the HJ equation can be considered as a classical limit of the Schrödinger equation (see, *e.g.*, Refs. 2, 3), and, when one solves the time-dependent Schrödinger equation (by separation of variables, in most cases), usually one does not obtain directly a general solution of this equation, but a family of solutions containing some parameters (or quantum numbers), $\alpha_1, \ldots, \alpha_n$,

$$\psi(q_i, t, \alpha_i), \tag{5}$$

which is, in this context, the analog of a complete solution of the HJ equation. Assuming that the wavefunctions (5) form a complete set [in the sense that any wavefunction can be expressed as a superposition of the wavefunctions (5)], the wavefunctions (5) are eigenfunctions of certain operators, P_i, with eigenvalues α_i, *i.e.*,

$$P_i \psi(q_j, t, \alpha_j) = \alpha_i \psi(q_j, t, \alpha_j). \tag{6}$$

As we shall show below, the operators P_i are constant, in the sense that

$$\frac{1}{\mathrm{i}\hbar}[P_i, H] + \frac{\partial P_i}{\partial t} = 0. \tag{7}$$

Furthermore, there exists a second set of n operators, Q_i, such that

$$Q_i \psi(q_j, t, \alpha_j) = \frac{\hbar}{\mathrm{i}} \frac{\partial \psi(q_j, t, \alpha_j)}{\partial \alpha_i} \tag{8}$$

[cf. Eq. (3)], which are also constant,

$$\frac{1}{\mathrm{i}\hbar}[Q_i, H] + \frac{\partial Q_i}{\partial t} = 0 \tag{9}$$

and these operators satisfy the commutation relations

$$[P_i, P_j] = 0, \quad [Q_i, Q_j] = 0, \quad [Q_i, P_j] = \mathrm{i}\hbar\delta_{ij} \qquad (10)$$

[cf. Eqs. (4)].

In other words, just as a complete solution of the HJ equation leads to $2n$ constants of motion, a solution (5) of the Schrödinger equation leads to $2n$ operators which are constants of motion.

In Sec. 2 we prove the validity of Eqs. (7), (9), and (10), and in Sec. 3 we present several examples. In the Appendix we obtain the constants of motion α_i, β_i arising from complete solutions of the HJ equation corresponding to the analogs in classical mechanics of the problems considered in Sec. 3. Throughout this paper we deal with wavefunctions in the coordinate representation.

2. Main results

Since we are assuming the completeness of the wavefunctions (5), Eqs. (6) and (8) do define some linear operators P_i and Q_i. In order to prove the validity of Eqs. (7), (9), and (10) we shall use the fact that if A and B are two linear operators such that $A\psi(q_i, t, \alpha_i) = B\psi(q_i, t, \alpha_i)$, for a complete set of wavefunctions $\psi(q_i, t, \alpha_i)$, then $A = B$.

We begin by applying the commutator $[P_i, H]$ to the wavefunction (5), and we make use of Eq. (6), the fact that P_i and H are linear operators, and that (5) is a solution of the time-dependent Schrödinger equation

$$\begin{aligned}[P_i, H]\psi(q_j, t, \alpha_j) &= P_i\left[\mathrm{i}\hbar\frac{\partial\psi(q_j, t, \alpha_j)}{\partial t}\right] - H\alpha_i\psi(q_j, t, \alpha_j) \\ &= \mathrm{i}\hbar\frac{\partial}{\partial t}\left[P_i\psi(q_j, t, \alpha_j)\right] - \mathrm{i}\hbar\left(\frac{\partial P_i}{\partial t}\right)\psi(q_j, t, \alpha_j) \\ &\quad - \alpha_i\mathrm{i}\hbar\frac{\partial\psi(q_j, t, \alpha_j)}{\partial t} = -\mathrm{i}\hbar\left(\frac{\partial P_i}{\partial t}\right)\psi(q_j, t, \alpha_j),\end{aligned}$$

thus proving the validity of Eq. (7).

Similarly, making use of Eq. (8) and the fact that H does not depend on the parameters α_i, we have

$$\begin{aligned}[Q_i, H]\psi(q_j, t, \alpha_j) &= Q_i\left[\mathrm{i}\hbar\frac{\partial\psi(q_j, t, \alpha_j)}{\partial t}\right] \\ &\quad - H\left[\frac{\hbar}{\mathrm{i}}\frac{\partial\psi(q_j, t, \alpha_j)}{\partial\alpha_i}\right] = \mathrm{i}\hbar\frac{\partial}{\partial t}\left[Q_i\psi(q_j, t, \alpha_j)\right] \\ &\quad - \mathrm{i}\hbar\left(\frac{\partial Q_i}{\partial t}\right)\psi(q_j, t, \alpha_j) - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_i}H\psi(q_j, t, \alpha_j) \\ &= -\mathrm{i}\hbar\left(\frac{\partial Q_i}{\partial t}\right)\psi(q_j, t, \alpha_j).\end{aligned}$$

Equations (10) can be proved in an analogous manner. For instance, using the fact that the P_i and Q_i are linear operators and that the P_i do not depend on the α_j,

$$\begin{aligned}[Q_i, P_j]\psi(q_k, t, \alpha_k) &= Q_i\left[\alpha_j\psi(q_k, t, \alpha_k)\right] \\ &\quad - P_j\frac{\hbar}{\mathrm{i}}\frac{\partial\psi(q_k, t, \alpha_k)}{\partial\alpha_i} = \alpha_j Q_i\psi(q_k, t, \alpha_k) \\ &\quad - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_i}\left[P_j\psi(q_k, t, \alpha_k)\right] = \alpha_j\frac{\hbar}{\mathrm{i}}\frac{\partial\psi(q_k, t, \alpha_k)}{\partial\alpha_i} \\ &\quad - \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_i}\left[\alpha_j\psi(q_k, t, \alpha_k)\right] = \mathrm{i}\hbar\delta_{ij}\psi(q_k, t, \alpha_k),\end{aligned}$$

hence, $[Q_i, P_j] = \mathrm{i}\hbar\delta_{ij}$.

3. Examples

In this section we give some examples where we explicitly find the conserved operators P_i and Q_i for some Hamiltonians.

3.1. Free particle

The usual Hamiltonian for a free particle of mass m in the three-dimensional space is

$$H = \frac{1}{2m}({p_1}^2 + {p_2}^2 + {p_3}^2),$$

where the p_i are the Cartesian components of the linear momentum. The wavefunctions

$$\begin{aligned}\psi(x, y, z, t, \alpha_1, \alpha_2, \alpha_3) = \exp\Bigg\{\frac{\mathrm{i}}{\hbar}\Bigg[\alpha_1 x \\ + \alpha_2 y + \alpha_3 z - \frac{1}{2m}({\alpha_1}^2 + {\alpha_2}^2 + {\alpha_3}^2)t\Bigg]\Bigg\} \qquad (11)\end{aligned}$$

are solutions of the corresponding time-dependent Schrödinger equation, containing three arbitrary parameters α_i. As we can see, Eq. (6) is satisfied by

$$P_i = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x_i}, \qquad (12)$$

that is, the operator P_i coincides with p_i.

On the other hand, a direct computation gives

$$\begin{aligned}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_i}\psi(x, y, z, t, \alpha_1, \alpha_2, \alpha_3) \\ = \left(x_i - \frac{\alpha_i t}{m}\right)\psi(x, y, z, t, \alpha_1, \alpha_2, \alpha_3), \qquad (13)\end{aligned}$$

and therefore,

$$Q_i = x_i - \frac{tp_i}{m}, \qquad (14)$$

where we have made use of Eq. (6). One readily verifies that the operators (12) and (14) indeed satisfy Eqs. (7), (9), and (10).

3.2. A time-dependent Hamiltonian

The time-dependent Schrödinger equation corresponding to the one-dimensional Hamiltonian

$$H = \frac{p^2}{2m} - ktx, \tag{15}$$

where k is a constant, is given by

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - ktx\psi \tag{16}$$

and admits solutions of the form [4]

$$\psi(x,t,\alpha) = \exp\left\{\frac{\mathrm{i}}{\hbar}\left[\alpha x + \frac{kt^2x}{2} - \frac{1}{2m}\left(\alpha^2 t + \frac{\alpha k t^3}{3} + \frac{k^2t^5}{20}\right)\right]\right\}, \tag{17}$$

where α is an arbitrary real number. According to the discussion above, we define an operator P by requiring that on the wavefunctions (17), $P\psi(x,t,\alpha) = \alpha\psi(x,t,\alpha)$ [cf. Eq. (6)]. Then, by inspection, one finds that

$$P = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x} - \frac{kt^2}{2} = p - \frac{kt^2}{2} \tag{18}$$

and one readily proves that this operator satisfies Eq. (7).

Now, defining an operator Q by the condition that, on the wavefunctions (17),

$$Q\psi(x,t,\alpha) = \frac{\hbar}{\mathrm{i}}\frac{\partial\psi(x,t,\alpha)}{\partial\alpha}$$

we find

$$Q = x - \frac{tp}{m} + \frac{kt^3}{3m}. \tag{19}$$

This operator is, indeed, a constant of motion, and a direct computation shows that $[Q,P] = \mathrm{i}\hbar$.

3.3. Particle in a uniform force field

The time-dependent Schrödinger equation corresponding to the Hamiltonian

$$H = \frac{1}{2m}({p_1}^2 + {p_2}^2 + {p_3}^2) + Fz, \tag{20}$$

where F is a constant, admits separable solutions of the form

$$\psi(x,y,z,t,\alpha_1,\alpha_2,\alpha_3) = \phi(z)\exp\left[\frac{\mathrm{i}}{\hbar}(\alpha_1 x + \alpha_2 y - \alpha_3 t)\right], \tag{21}$$

where the α_i are three arbitrary parameters and ϕ is a solution of the Airy equation

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}w^2} - w\phi = 0,$$

where

$$w \equiv \left(\frac{2mF}{\hbar^2}\right)^{1/3}\left(z - \frac{\alpha_3}{F} + \frac{{\alpha_1}^2 + {\alpha_2}^2}{2mF}\right). \tag{22}$$

One can readily find that the operators P_i defined by Eq. (6) are

$$P_1 = p_1, \qquad P_2 = p_2, \qquad P_3 = H. \tag{23}$$

Note that even though the wavefunctions (21) satisfy

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,y,z,t,\alpha_1,\alpha_2,\alpha_3) = \alpha_3\psi(x,y,z,t,\alpha_1,\alpha_2,\alpha_3),$$

it would be wrong to say that P_3 is equal to $\mathrm{i}\hbar\partial/\partial t$ because the latter has no meaning on an arbitrary wavefunction, since an arbitrary wavefunction is not a function of t. (Similarly, $\partial/\partial\alpha_i$ is not an operator defined on an arbitrary wavefunction.)

In order to identify the operators Q_i, which are defined by Eq. (8), we observe that, by virtue of the chain rule and Eq. (22),

$$\frac{\partial\phi}{\partial\alpha_1} = \frac{\alpha_1}{mF}\frac{\partial\phi}{\partial z},$$

hence

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_1}\psi(x,y,z,t,\alpha_1,\alpha_2,\alpha_3) = \left(x + \frac{\alpha_1 p_3}{mF}\right)\psi(x,y,z,t,\alpha_1,\alpha_2,\alpha_3)$$

and therefore

$$Q_1 = x + \frac{p_1 p_3}{mF}. \tag{24}$$

In a similar manner one finds that

$$Q_2 = y + \frac{p_2 p_3}{mF}, \qquad Q_3 = -t - \frac{p_3}{F}. \tag{25}$$

As in the previous examples, one can verify directly that the operators P_i and Q_i satisfy Eqs. (7), (9), and (10).

3.4. Final remarks

It should be clear that, in many cases, it may be difficult to find the operators P_i, Q_i explicitly. For instance, in the case of a particle in a central potential in two dimensions, the Schrödinger equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}\right] + V(r)\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t},$$

admits separable solutions of the form

$$\psi(r,\theta,t,\alpha_1,\alpha_2) = \phi(r)\exp\left[\frac{\mathrm{i}}{\hbar}(\alpha_1\theta - \alpha_2 t)\right]. \tag{26}$$

Then, one readily finds that

$$P_1 = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\theta}, \qquad P_2 = H.$$

On the other hand,

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\alpha_1}\psi(r,\theta,t,\alpha_1,\alpha_2) = \theta\psi(r,\theta,t,\alpha_1,\alpha_2) + \frac{\partial\phi}{\partial\alpha_1}\exp\left[\frac{\mathrm{i}}{\hbar}(\alpha_1\theta - \alpha_2 t)\right],$$

but we are unable to express the last term as some linear operator made out of r, θ and their conjugate momenta acting on the wavefunction (26), though we could always give an integral representation for P_i or Q_i making use of the assumed completeness of the wavefunctions (5).

This example also illustrates the fact that we can consider parameters α_i belonging to a discrete spectrum or to a continuous one (as in the first three examples above).

4. Conclusions

As we have shown, apart from its usual interpretation, the solutions of the Schrödinger equation containing n arbitrary parameters are analogous to the complete solutions of the HJ equation, defining $2n$ conserved operators. In a similar manner as a complete solution of the HJ equation yields the solution of the Hamilton equations in classical mechanics, a solution of the Schrödinger equation containing n arbitrary parameters leads to the solutions of the Heisenberg equations.

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Appendix

In this appendix we consider the analogs in classical mechanics of the systems employed in Sec. 3. We find the constants of motion associated with complete solutions of the corresponding HJ equation in order to compare them with the operators P_i, Q_i obtained above.

The function

$$S(x,y,z,t,\alpha_1,\alpha_2,\alpha_3) = \alpha_1 x + \alpha_2 y + \alpha_3 z - \frac{1}{2m}({\alpha_1}^2 + {\alpha_2}^2 + {\alpha_3}^2)t \qquad \text{(A1)}$$

is a complete solution of the HJ equation for a free particle in Cartesian coordinates. Making use of Eqs. (2) and (3) we find the constants of motion α_i and β_i given by

$$\alpha_i = p_i, \qquad \beta_i = x_i - \frac{\alpha_i t}{m} = x_i - \frac{p_i t}{m} \qquad \text{(A2)}$$

[cf. Eqs. (12) and (14)].

In the case of the time-dependent Hamiltonian (15) a complete solution of the corresponding HJ equation is given by [4]

$$S(x,t,\alpha) = \alpha x + \frac{kt^2 x}{2} - \frac{1}{2m}\left(\alpha^2 t + \frac{\alpha k t^3}{3} + \frac{k^2 t^5}{20}\right) \qquad \text{(A3)}$$

[cf. Eq. (17)]. This functions yields the constants of motion

$$\alpha = p - \frac{kt^2}{2}, \qquad \beta = x - \frac{pt}{m} + \frac{kt^3}{3m}, \qquad \text{(A4)}$$

which have the same form as the operators P and Q given by Eqs. (18) and (19), respectively.

The HJ equation corresponding to the Hamiltonian for a particle in a uniform force field (20) admits solutions of the form

$$S(x,y,z,t,\alpha_1,\alpha_2,\alpha_3) = \alpha_1 x + \alpha_2 y - \alpha_3 t + f(z),$$

where the α_i are arbitrary parameters and

$$f(z) = \pm \int \sqrt{2m(\alpha_3 - Fz) - {\alpha_1}^2 - {\alpha_2}^2}\,\mathrm{d}z.$$

With the aid of formulas (2) and (3), noting that

$$\frac{\partial f}{\partial \alpha_1} = \frac{\alpha_1}{mF}\frac{\partial f}{\partial z}, \qquad \frac{\partial f}{\partial \alpha_2} = \frac{\alpha_2}{mF}\frac{\partial f}{\partial z}, \qquad \frac{\partial f}{\partial \alpha_3} = -\frac{1}{F}\frac{\partial f}{\partial z},$$

one finds that the constants of motion α_i, β_i are

$$\alpha_1 = p_1, \qquad \alpha_2 = p_2, \qquad \alpha_3 = H,$$
$$\beta_1 = x + \frac{p_1 p_3}{mF}, \qquad \beta_2 = y + \frac{p_2 p_3}{mF}, \qquad \beta_3 = -t - \frac{p_3}{F},$$

which have the same form as the conserved operators (23)–(25).

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